SYNTHESIS AND ELUCIDATION OF STRUCTURE OF 1- OR 2-R-3-R',R"-AMINO-5-AMINO-1,2,4-TRIAZOLES

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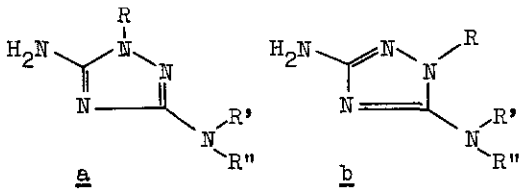
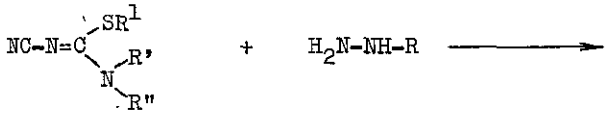
The reaction of N-cyano-S-R^1-N'-R',R"-isothiourea (1) with hydrazine (2, R=H) or substituted hydrazines (2, R=alkyl, aralkyl) can lead in case of R',R" ≠ H to a, b or c type 3-R',R"-amino-5-amino-1,2,4-triazole derivatives, while in case of R'=H, R"≠H the d, e and f tautomeric forms must be taken in account, too.

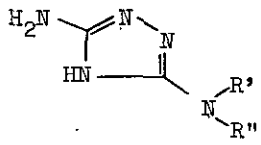


a b

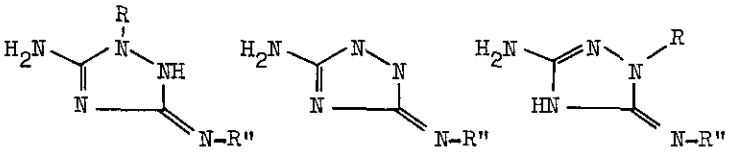


1, R^1= alkyl, aralkyl
R',R"= H, alkyl, aralkyl, aryl

2, R= H, CH_3, CH_2Ph



c
(only if R=H)



d e f
(only if R'=H)

The isomeric and tautomeric structure of products obtained with different R, R' and R" substituents was proved on the basis of their IR, UV, ^{1}H-NMR and ^{13}C-NMR spectra with the help of the spectra of the corresponding Schiff bases as well as the corresponding 3-alkylthio-1,2,4-triazoles of proved structure (1,2).

References:

(1) J. Reiter, Topics in Chemistry of Heterocyclic Compounds (Bratislava), 1981, pp. 58-80.
(2) J. Reiter et al., J. Heterocyclic. Chem. 19, 1157-64 (1982).